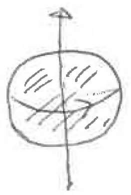
(6) Spin Angular Momentum: An application

$\vec{J}$: "Total" ang. mom.
$\vec{L}$: "orbital" "
$\vec{S}$: "spin" "

→ $\boxed{\text{Magnetic Resonance}}$

* Spin : the historical origin.

∘ Classical picture : Not correct at all, but it's convenient.
totally wrong, actually.

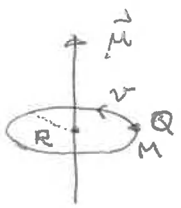


"self-spinning ball" : If it has a charge, it produces a magnetic moment.

(Goudsmit, Uhlenbeck 1925 ; Kronig)

c.f. Stern - Gerlach exp. : 1922.
Pauli's formalism : 1927.

an orbiting charge



→ The magnetic moment

$$\vec{\mu} = \frac{I\vec{A}}{c} \Rightarrow \mu = \frac{Q}{2\pi R}v \cdot \frac{\pi R^2}{c} = \frac{Q}{2c}Rv$$

$$= \frac{Q}{2Mc}L \qquad \| \; L = MRv$$

$$\therefore \quad \frac{\mu}{L} = \frac{Q}{2Mc}$$

gyromagnetic ratio   independent of R, and v.

→ ~ quantum analog of orbital ang. momentum
(magnetic moment.

What about the electron ?

a self-spinning ball ⟶ $\vec{\mu} \overset{?}{=} \frac{e}{2m_e c}\vec{S}$ $\| \; e<0$

Rubbish !!!   • An electron doesn't have any "size"!
• To reproduce $S = \frac{\hbar}{2}$, $v \gg c$!
(if we put the classical electron radius : $\frac{e^2}{m_e c^2}$)

• and $\frac{\mu}{S} = \frac{e}{m_e c}$ in exp.
"not" $\frac{e}{2m_e c}$.

Despite all the bad assumptions and non-sense

$$\vec{\mu} = g \frac{e}{2mc} \vec{S}$$

works very well with some factor "g" (electron : $g \approx 2$)

To understand this,

you need "fully relativistic" QM.

QED

Spin in a Magnetic field : Hamiltonian

$$H = -\vec{\mu} \cdot \vec{B} = -\gamma \vec{S} \cdot \vec{B}$$

where

"gyromagnetic ratio"

$$\gamma_e = -g_e \frac{|e|}{2m_e c} \quad \text{with } g_e \simeq 2 \text{ for an electron.}$$

$$\gamma_p = g_p \frac{|e|}{2m_p c} \quad \text{with } g_p \simeq 5.6 \text{ for a proton}$$

$$\gamma_n = g_n \frac{|e|}{2m_p c} \quad \text{with } g_n \simeq -3.8 \text{ for a neutron}$$

This one is charge - neutral!

NOTE : $m_p \approx m_n \gg m_e$ (1000 times larger)

for a nucleus $\quad \gamma = g \frac{|e|}{2m_p c} = g \frac{\mu_N}{\hbar}$

$\parallel \quad \mu_N$ = nuclear magneton $= \frac{|e|}{2m_p c}$.

(^1H, ^{13}C, ^{19}F, ...)

* A spin-$\frac{1}{2}$ particle in a periodic magnetic field

: The rotating frame

$$\vec{B} = B_0 \hat{z} + B_1 (\hat{x} \cos\omega t - \hat{y} \sin\omega t).$$

$\parallel \quad \omega_0 = \gamma B_0$, $\quad \omega_1 = \gamma B_1$

$$H = -\vec{\mu} \cdot \vec{B}$$

"Rabi" frequency

$$= -\frac{\hbar}{2} \omega_0 \sigma_3 - \frac{\hbar}{2} \omega_1 (\sigma_1 \cos\omega t - \sigma_2 \sin\omega t)$$

Schrödinger equation : $i\hbar \frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle$

But, now H is time-dependent !

$\uparrow$
χ (Pauli's formalism)

- Rotating frame :

$$\chi_R = U_R\, \chi \qquad \| \quad U_R \equiv U(t)$$

→ Schrödinger eq. (in the Pauli's formalism)

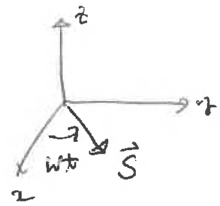
$$i\hbar \frac{\partial}{\partial t}\left(U_R^{\dagger} \chi_R\right) = H\, U_R^{\dagger} \chi_R$$

$$i\hbar \left(\frac{\partial}{\partial t} U_R^{\dagger}\right) \chi_R + i\hbar\, U_R^{\dagger}\left(\frac{\partial}{\partial t} \chi_R\right) = H\, U_R^{\dagger} \chi_R$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} \chi_R = \underline{i\hbar\, U_R \frac{\partial}{\partial t} U_R^{\dagger}}\, \chi_R$$

$$+ \underline{U_R H U_R^{\dagger}}\, \chi_R$$

$$\equiv \underline{H_R}\, \chi_R .$$



The 2nd term in RHS :

$$U_R\left[-\frac{\hbar}{2}\omega_0 \sigma_3 - \frac{\hbar}{2}\omega_1\left(\sigma_1 \cos\omega t - \sigma_2 \sin\omega t\right)\right] U_R^{\dagger}$$

We know : $= e^{i\sigma_3 \frac{\omega t}{2}}\, \sigma_1\, e^{-i\sigma_3 \frac{\omega t}{2}}$
from the spin precession.

Thus, if we choose $U_R = \exp\left[-i\sigma_3 \frac{\omega t}{2}\right]$

$$= \underline{-\frac{\hbar}{2}\left[\omega_0 \sigma_3 + \omega_1 \sigma_1\right]}$$

no t-dep.

The 1st term in RHS :

$$i\hbar\, U_R \frac{\partial}{\partial t} U_R^\dagger = \frac{\hbar}{2}\omega\sigma_3 \quad \Big\| \quad \text{We choose } U_R = e^{-i\sigma_3\frac{\omega t}{2}}$$

$\Rightarrow$ Schrödinger eq.

$$i\hbar \frac{\partial}{\partial t}\chi_R = \frac{\hbar}{2}\left[(\omega-\omega_0)\sigma_3 - \omega_1\sigma_1\right]\chi_R \equiv \frac{\hbar}{2}A\,\chi_R$$

$\delta \equiv (\omega-\omega_0)$: "detuning" $\quad \Big\| \quad A = \begin{bmatrix} \delta & -\omega_1 \\ -\omega_1 & -\delta \end{bmatrix}$

Sol. $\quad \chi_R(t) = \exp\left[-i\frac{A}{2}t\right]\chi_R(0)$

diagonalization of A $\quad A = U\begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}U^\dagger \quad \Big\| \quad \Omega = \sqrt{\delta^2+\omega_1^2}$

where $\quad U = \frac{1}{\sqrt{2\Omega(\Omega+\delta)}}\begin{pmatrix} \Omega+\delta & \omega_1 \\ -\omega_1 & \Omega+\delta \end{pmatrix}$

when $\chi_R(0) = \chi_\uparrow = \binom{1}{0}$

$$\Rightarrow \chi_R(t) = \frac{1}{2\Omega(\Omega+\delta)}\begin{bmatrix} (\Omega+\delta)^2 e^{-i\frac{\Omega}{2}t} + \omega_1^2 e^{i\frac{\Omega}{2}t} \\ -\omega_1(\Omega+\delta)e^{-i\frac{\Omega}{2}t} + \omega_1(\Omega+\delta)e^{i\frac{\Omega}{2}t} \end{bmatrix}$$

$$\therefore \langle\uparrow|\chi_R\rangle = \cos\frac{\Omega}{2}t - i\frac{\delta}{\Omega}\sin\frac{\Omega}{2}t.$$

$$\langle\downarrow|\chi_R\rangle = \frac{i\omega_1}{\Omega}\sin\frac{\Omega}{2}t.$$

. prob. finding the spin in the state $|\downarrow\rangle$

$$P_\downarrow(t) = \frac{\omega_1^2}{\Omega^2}\sin^2\frac{\Omega}{2}t,$$

"Rabi" Oscillations "

. max. prob.

$\rightarrow$ MRI, NMR

$$P_\downarrow^{max} = \frac{\omega_1^2}{\omega_1^2 + \underbrace{(\omega-\omega_0)^2}_{=\delta}}$$

: resonance curve of width ω_1.

(17) Orbital Angular Momentum

- Generator of rotations in CM : $\vec{L} = \vec{x} \times \vec{p}$
- Let's check if $\vec{L} = \tilde{x} \times \tilde{p}$ works for QM, too.

① <u>fundamental commutation relation</u> : $[L_i, L_j] = i\epsilon_{ijk} L_k$

- useful commutation relations.

$$[L_i, \tilde{x}_j] = \epsilon_{lmi} [\tilde{x}_l \tilde{p}_m , \tilde{x}_j] = \epsilon_{lmi} \tilde{x}_l [\tilde{p}_m, \tilde{x}_j]$$

$$= -i\hbar \, \epsilon_{lmi} \tilde{x}_l \delta_{mj} = \underline{i\hbar \, \epsilon_{ijk} \tilde{x}_k} \; !$$

Similarly,

$$[L_i, \tilde{p}_j] = i\hbar \, \epsilon_{ijk} \tilde{p}_k .$$

- $$[L_i, L_j] = \epsilon_{lmj} [L_i, \tilde{x}_l \tilde{p}_m]$$

$$= \epsilon_{lmj} \left(\tilde{x}_l [L_i, \tilde{p}_m] + [L_i, \tilde{x}_l] \tilde{p}_m \right)$$

$$= i\hbar \, \epsilon_{lmj} \left(\epsilon_{im\mu} \tilde{x}_l \tilde{p}_\mu + \epsilon_{il\nu} \tilde{x}_\nu \tilde{p}_m \right)$$

$$= i\hbar \left[(\delta_{li}\delta_{j\mu} - \delta_{l\mu}\delta_{ji}) \tilde{x}_l \tilde{p}_\mu + (\delta_{m\nu}\delta_{ji} - \delta_{mi}\delta_{j\nu}) \tilde{x}_\nu \tilde{p}_m \right]$$

$$= i\hbar \left[\tilde{x}_i \tilde{p}_j - \tilde{x}_j \tilde{p}_i \right] = \underline{i\hbar \, \epsilon_{ijk} L_k} \quad //$$

* NOTE : Product of two Levi-Civita symbols.

$$\epsilon_{ijk}\epsilon_{lmn} = \delta_{il}\delta_{jm}\delta_{kn} + \delta_{im}\delta_{jn}\delta_{kl} + \delta_{in}\delta_{jl}\delta_{km} - \delta_{im}\delta_{jl}\delta_{kn} - \delta_{il}\delta_{jn}\delta_{km} - \delta_{in}\delta_{jm}\delta_{kl} .$$

if $i = l$, $\underline{\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}}$.

- $(\vec{a} \times \vec{b})_k = \epsilon_{ijk} a_i b_j$, $\det[A] = \epsilon_{ijk} a_{1i} a_{2j} a_{3k}$.

(3×3 matrix)

② Infinitesimal Rotations : δa about a fixed axis.

→ Matrix representation

i) δa about $\hat{z}$-axis

$$\left[1-\frac{i}{\hbar}\delta a L_z\right]|x,y,z\rangle = \left[1-\frac{i}{\hbar}\delta a\,(\tilde{x}\tilde{p}_y-\tilde{y}\tilde{p}_x)\right]|x,y,z\rangle$$

$$= \left[1-\frac{i}{\hbar}\tilde{p}_x(-\delta a\cdot y)-\frac{i}{\hbar}\tilde{p}_y(\delta a\cdot x)\right]|x,y,z\rangle$$

$$= |x-\delta a\cdot y,\ y+\delta a\cdot x,\ z\rangle$$ ⇒ This is indeed the rot. $|R_{\hat{z}}(\delta a)\vec{x}\rangle$.

For $|\alpha\rangle$, an arbitrary ket of a spinless particle,

$$\langle x,y,z|\left[1-\frac{i}{\hbar}\delta a L_z\right]|\alpha\rangle = \langle x+\delta a\, y,\ y-\delta a\, x,\ z\,|\,\alpha\rangle \quad \cdots (*)$$

$$\hookrightarrow = \left[\left(1+\frac{i}{\hbar}\delta a L_z\right)|x,y,z\rangle\right]^{\dagger}$$

In terms of a wave function,

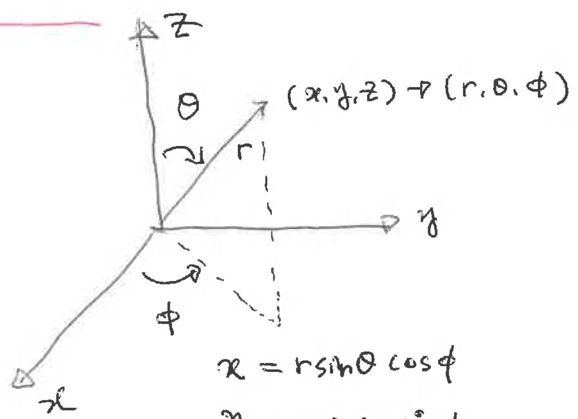
$$\Psi_{R\alpha}(\vec{x}) = \Psi_\alpha(R^{-1}\vec{x}).$$

* Representation of L_z in the position space (spherical coordinates)

$(*) \Rightarrow \langle x,y,z|\alpha\rangle \longrightarrow \langle r,\theta,\phi|\alpha\rangle$

rotation

$\theta \to \theta+\delta\theta, \quad \phi\to\phi+\delta\phi$



$\delta x = r\cos\theta\cos\phi\,\delta\theta - r\sin\theta\sin\phi\,\delta\phi$

$\delta y = r\cos\theta\sin\phi\,\delta\theta + r\sin\theta\cos\phi\,\delta\phi$

$\delta z = -r\sin\theta\,\delta\theta.$

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$